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PARALLEL PROJECTED VARIABLE METRIC ALGORITHMS FOR UNCONSTRAINED OPTIMIZATION

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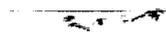
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FOR UNCONSTRAINED OPTIMIZATION

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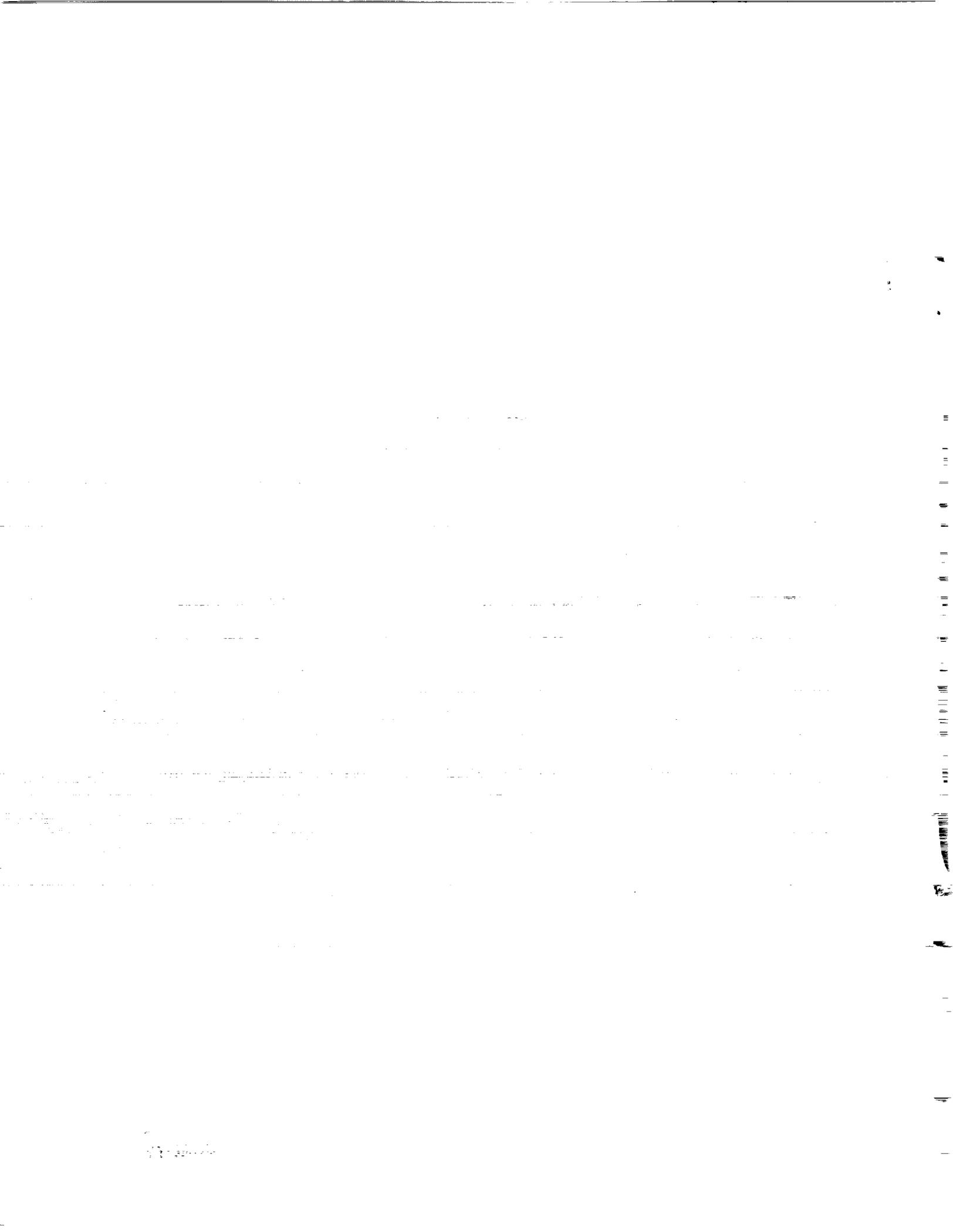
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ABSTRACT

We review the parallel variable metric optimization algorithms of Straeter (1973) and van Laarhoven (1985) and point out the possible drawbacks of these algorithms. By including Davidon (1975) projections in the variable metric updating we can generalize Straeter's algorithm to a family of parallel projected variable metric algorithms which do not suffer the above drawbacks and which retain quadratic termination. Finally we consider the numerical performance of one member of the family on several standard example problems and illustrate how the choice of the displacement vectors affects the performance of the algorithm.

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1 Introduction

In this paper we consider the problem of finding the unconstrained minimum of the nonlinear function of n variables $f(\mathbf{x})$, where $f(\mathbf{x})$ is twice continuously differentiable and $\mathbf{x} \in \mathbb{R}^n$. In particular we consider the development of algorithms for the solution of the problem on a parallel computer. Function and gradient evaluations are usually considered to be the most computationally expensive part of an optimization algorithm and most parallel optimization algorithms include the simultaneous evaluation of the function, or the gradient vector, at a number of different points. The expectation is that this extra function or gradient information will result in an algorithm which converges more rapidly. For a survey of parallel optimization algorithms see Lootsma and Ragsdell (1988), Lootsma (1989) or Schnabel (1988).

On a sequential computer, when the function $f(\mathbf{x})$ and the gradient vector $\mathbf{g}(\mathbf{x})$ are available, but the Hessian matrix $\mathbf{G}(\mathbf{x})$ is not available, one of the most popular methods for finding an unconstrained local minimum is a variable metric (quasi-Newton) method (see Fletcher (1987), Gill, Murray and Wright (1981), Dennis and Schnabel (1983)). One way of adapting such an algorithm to a parallel computer is that considered by Straeter (1973) and van Laarhoven (1985). It is the further development of these ideas which is the subject of this paper. Alternative approaches to parallel variable metric methods have been suggested by Schnabel (1987) and Byrd, Schnabel and Shultz (1988a,b).

In Section 2 we review the parallel variable metric method of Straeter (1973) and van Laarhoven (1985) and point out the possible drawbacks of the method. One way of avoiding these difficulties is to use suitably projected vectors in the variable metric updating, as suggested by Davidon (1975) in the context of a sequential variable metric algorithm. This leads to the family of parallel variable metric methods described in Section 3. In Section 4 we consider the numerical performance of these new algorithms on a collection of test examples.

2 A parallel symmetric rank one algorithm

The first attempt to develop a parallel variable metric algorithm is due to Straeter (1973). He proposed a parallel generalisation of the well-known symmetric rank-one (*SR1*) algorithm (see Fletcher (1987), p.51). On each iteration the algorithm evaluates the gradient vector at different displaced points, *in parallel*, and incorporates the gradient information thus obtained into the approximate inverse Hessian matrix \mathbf{H} by a sequence of *SR1* updates. The expectation, which is justified by limited numerical experiments, is that this extra gradient information will result in an improved Hessian approximation which in turn will

result in an algorithm which requires fewer iterations for convergence.

If we let H denote the approximate inverse Hessian matrix, then Straeter's algorithm is given by the following steps.

1. Select $\mathbf{x}\lambda_0 \in \mathfrak{R}\lambda_n$, and n linearly independent directions $\delta\lambda_1, \delta\lambda_2, \dots, \delta\lambda_n$, and set $H_0 = I$ and $k = 0$.
2. Calculate, IN PARALLEL, $\nabla f(\mathbf{x}\lambda_k), \nabla f(\mathbf{x}\lambda_{k,1}), \nabla f(\mathbf{x}\lambda_{k,2}), \dots, \nabla f(\mathbf{x}\lambda_{k,n})$, where $\mathbf{x}\lambda_{k,j} = \mathbf{x}\lambda_k + \delta\lambda_j$.

With $V_{k,0} = H_k$, for $j = 1, 2, \dots, n$, calculate

$$\gamma\lambda_{k,j} = \nabla f(\mathbf{x}\lambda_{k,j}) - \nabla f(\mathbf{x}\lambda_k), \quad (2.1)$$

$$\tau\lambda_{k,j} = V_{k,j-1}\gamma\lambda_{k,j} - \delta\lambda_j, \quad (2.2)$$

$$V_{k,j} = V_{k,j-1} - \frac{\tau\lambda_{k,j}\tau\lambda_{k,j}\lambda^T}{\gamma\lambda_{k,j}\lambda^T\tau\lambda_{k,j}}. \quad (2.3)$$

Set $H_{k+1} = V_{k,n}$ and calculate the search direction

$$s\lambda_k = -H_{k+1}\nabla f(\mathbf{x}\lambda_k). \quad (2.4)$$

3. Perform an approximate line search along $s\lambda_k$ to determine the steplength $\alpha\lambda_k$. Set

$$\mathbf{x}\lambda_{k+1} = \mathbf{x}\lambda_k + \alpha\lambda_k s\lambda_k, \quad (2.5)$$

$$k = k + 1 \quad (2.6)$$

and return to 2.

It can be shown that, for the positive definite quadratic function $q(\mathbf{x}) = \frac{1}{2}\mathbf{x}\lambda^T A \mathbf{x} + b\lambda^T \mathbf{x} + c$ and for an arbitrary initial point $\mathbf{x}\lambda_0$, $H_1 = A\lambda^{-1}$ and the first iteration will locate the minimum of $q(\mathbf{x})$ provided that a steplength of 1 is chosen. This result is to be expected since the *SR1* algorithm is known to generate the true (inverse) Hessian matrix after inexact line searches along n linearly independent directions (see Brodijć (1977)).

The *SR1* updates (step 2) of Straeter's algorithm are performed sequentially, with $V_{k,j}$ dependent on $\delta\lambda_j, \gamma\lambda_{k,j}$ and $V_{k,j-1}$. It is not possible to incorporate these updates simultaneously since it can be shown that multiple secant updates are, in general, inconsistent with preserving symmetry of the approximate matrices (see Schnabel (1983)).

van Laarhoven (1985) attempts to generalize Straeter's ideas to the Huang family of updating formulae (Huang (1970)), but finds that, in general, the only symmetric formula

which has quadratic termination is Straeter's parallel *SR1* formula. This is inevitable since the *SR1* formula is the only member of the Broyden family of updating formulae which has quadratic termination without exact line searches (see Brodlie (1977)).

van Laarhoven (1985) derives a parallel generalisation of Broyden's rank one formula (Broyden (1965)). This results in an algorithm which has quadratic termination, but the approximate matrices are in general unsymmetric.

One major drawback of the parallel algorithms of this section is that the approximate matrices H_k are not guaranteed to be positive definite and may fail to exist if the denominator of the rank one correction is zero. In the next section we describe a parallel generalisation of Davidon's projected updating formula (Davidon (1975)) which has quadratic termination and which guarantees the existence and positive definiteness of the approximate matrices.

3 A family of parallel symmetric rank two algorithms

In this section we obtain a family of parallel symmetric rank two algorithms, which have quadratic termination, by generalising Straeter's ideas to the family of projected updating formulae of Davidon (1975). Serial variable metric algorithms based on Davidon's projected updating formulae can be shown to have quadratic termination without requiring exact line searches on each iteration.

The obvious extension of Straeter's ideas would be to use a projected updating formula to update $V_{k,j}$, $j = 0, 1, \dots, n-1$, (and thus H_k) in step 2 of the algorithm of Section 2. However to calculate the required projected vectors it is necessary to also update the inverse matrices $V_{k,j}^{-1}$, $j = 0, 1, \dots, n$. This contrasts with the serial implementation where the special form of the gradient differences enables the projected vectors to be calculated without explicit knowledge of $H_{\lambda-1}$ (see Davidon (1975), Shanno and Phua (1978a) and Freeman and Körner (1982)). Given that both the approximate Hessian matrix and its inverse are required it is efficient to update the LDL^T factors of an approximation B to the Hessian matrix itself.

In addition, since the information is readily available, we use the same formula to update the approximate Hessian matrix after each line search. The resulting algorithm is as follows.

1. Select $x_{\lambda_0} \in \mathbb{R}^n$, and n linearly independent directions $\delta_{\lambda_1}, \delta_{\lambda_2}, \dots, \delta_{\lambda_n}$, and set $B_0 = I$ ($\Rightarrow L_0 = I$ and $D_0 = I$) and $k = 0$, and calculate $\nabla f(x_{\lambda_0})$.
2. Calculate, IN PARALLEL, $\nabla f(x_{\lambda_k, 1}), \nabla f(x_{\lambda_k, 2}), \dots, \nabla f(x_{\lambda_k, n})$, where $x_{\lambda_k, j} = x_{\lambda_k} + \delta_{\lambda_j}$

With $W_{k,0} = L_k D_k L_k^T = B_k$, for $j = 1, 2, \dots, n$, calculate

$$\gamma_{\lambda_k, j} = \nabla f(x_{\lambda_k, j}) - \nabla f(x_{\lambda_k}), \quad (3.1)$$

and update the $LDL\lambda T$ factors of $W_{k,j-1} \rightarrow W_{k,j}$ using a projected symmetric rank two updating formula.

Set $\bar{L}_{k+1}\bar{D}_{k+1}\bar{L}_{k+1}\lambda T = \bar{B}_{k+1} = W_{k,n}$ and calculate the search direction $s\lambda k$, where

$$\bar{L}_{k+1}\bar{D}_{k+1}\bar{L}_{k+1}\lambda T s\lambda k = -\nabla f(x\lambda k). \quad (3.2)$$

3. Perform an approximate line search along $s\lambda k$ to determine the steplength $\alpha\lambda k$. Set

$$x\lambda k + 1 = x\lambda k + \alpha\lambda k s\lambda k, \quad (3.3)$$

calculate $\nabla f(x\lambda k + 1)$ and

$$\gamma\lambda k = \nabla f(x\lambda k + 1) - \nabla f(x\lambda k), \quad (3.4)$$

and update the $LDL\lambda T$ factors of $\bar{B}_{k+1} \rightarrow B_{k+1}$ using a projected symmetric rank two updating formula. Set

$$L_{k+1}D_{k+1}L_{k+1}\lambda T = B_{k+1}, \quad (3.5)$$

$$k = k + 1 \quad (3.6)$$

and return to 2.

If we omit the superfixes and suffices and let \sharp denote an updated quantity then the projected rank two updating formula for W is given by

$$W\lambda\sharp = W + \frac{yy\lambda T}{y\lambda Tz} - \frac{Wz z\lambda T W}{z\lambda T W z} + \phi(z\lambda T W z)ww\lambda T, \quad (3.7)$$

where

$$w = \frac{y}{y\lambda Tz} - \frac{Wz}{z\lambda T W z}, \quad (3.8)$$

$$y = P\gamma, \quad (3.9)$$

$$z = P\lambda T\delta, \quad (3.10)$$

$$P = Y[Y\lambda T W \lambda^{-1} Y]\lambda^{-1} Y\lambda T W \lambda^{-1}, \quad (3.11)$$

$$Y = [u, v], \quad (3.12)$$

and v is given by

$$v = W\delta - \gamma, \quad (3.13)$$

and $u\lambda\sharp$, one of the basis vectors for the next application of the updating formula, is given by

$$u\lambda\sharp = (v\lambda T\delta)u - (u\lambda T\delta)v. \quad (3.14)$$

If we set $\mathbf{u} = -\nabla f(\mathbf{x} \lambda k)$ at the start of each iteration then the algorithm can be shown to have quadratic termination (see Davidon (1975), Powell (1977)). Further, provided that $\mathbf{y} \lambda T \mathbf{z} > 0$ and ϕ is suitably bounded below, the update maintains both symmetry and positive definiteness of $W_{k,j}$ and hence B_k .

We update the LDL^T factors of $W_{k,j}$ by using the formulae given in Fletcher and Powell (1974). Their composite t-method includes monitoring of the updating to ensure that rounding errors do not cause the matrices $W_{k,j}$ to become indefinite.

As noted in Freeman and Körner (1982), the vectors \mathbf{u} and \mathbf{v} simply provide a basis for a space which is orthogonal to the preceding updating directions. In order to make this basis well-scaled we normalise the vectors \mathbf{u} and \mathbf{v} in the $W \lambda^{-1}$ metric, so that we define the normalised basis vectors

$$\bar{\mathbf{u}} = \frac{\mathbf{u}}{(\mathbf{u} \lambda T W \lambda^{-1} \mathbf{u}) \lambda^{\frac{1}{2}}} \quad (3.15)$$

$$\bar{\mathbf{v}} = \frac{\mathbf{v}}{(\mathbf{v} \lambda T W \lambda^{-1} \mathbf{v}) \lambda^{\frac{1}{2}}} \quad (3.16)$$

and use these vectors in place of \mathbf{u} and \mathbf{v} in (3.12).

When $\bar{\mathbf{u}}$ and $\bar{\mathbf{v}}$ are linearly dependent in the $W \lambda^{-1}$ metric the projected symmetric rank two update reduces to the symmetric rank one (SR1) update. Thus if

$$1 - (\bar{\mathbf{u}} \lambda T W \lambda^{-1} \bar{\mathbf{v}}) \lambda^2 < \epsilon \quad (3.17)$$

where ϵ is the machine precision, then a symmetric rank one update, based on γ and δ , is attempted. Similarly, if

$$\mathbf{y} \lambda T \mathbf{z} < \epsilon, \quad (3.18)$$

the projected symmetric rank two update is not guaranteed to maintain positive definiteness and a symmetric rank one update, based on γ and δ , is again attempted. In both cases this SR1 update is abandoned if it would result in an indefinite Hessian matrix, a condition which can be recognised by the composite t-method which is used to perform the updating.

4 Numerical Results

In this section we illustrate the numerical performance of the algorithm of Section 3 by applying it to the set of test problems considered by Shanno and Phua (1978a). The results were obtained using the Amdahl 5890-300 at the Manchester Computing Centre using about 14 decimal digit accuracy. Before considering the numerical results some of the details of the algorithm need to be clarified.

The line search of step 3. uses bracketing and interpolation as described in Section 2.6 of Fletcher (1987) with the parameters $\sigma = 0.99$ and $\rho = 0.01$. The convergence condition of the overall algorithm is

$$\|\delta\lambda_k\|_2 \leq \epsilon, \quad (4.1)$$

where in the examples of this section we take $\epsilon = 10\lambda - 7$, or approximately the square root of the machine precision. The parameter ϕ of (3.7) is taken to be 0 corresponding to a projected BFGS updating formula.

We consider two alternative choices for the n linearly independent directions $\delta\lambda_j, j = 1, 2, \dots, n$, of step 2. of the algorithm.

The algorithm, *PARALLEL I*, defines $\delta\lambda_j$ as

$$\delta\lambda_j = \tau e\lambda_j, \quad (4.2)$$

where $e\lambda_j$ is the $j\lambda th$ column of the $n \times n$ identity matrix, and

$$\tau = \begin{cases} \mu, & k = 0, \\ \mu \|\mathbf{x}\lambda_k - \mathbf{x}\lambda_{k-1}\|_2, & k \geq 1 \end{cases} \quad (4.3)$$

Thus on the $k\lambda th$ iteration the magnitudes of the displacements on which the parallel updating is based depend on the magnitude of the step taken by the algorithm on the $(k-1)\lambda th$ iteration. In the examples of Table 1 we take $\mu = 10\lambda - 2$, except for the extended Rosenbrock function with $n = 20$, in which case we take $\mu = 10\lambda - 4$.

The alternative algorithm, *PARALLEL II*, defines

$$\delta\lambda_j = \tau l\lambda_j / \|l\lambda_j\|_2, \quad (4.4)$$

where, on the $k\lambda th$ iteration, $l\lambda_j$ is the $j\lambda th$ column of the $n \times n$ matrix $L_k\lambda - T$ and τ is given by (4.3). The justification for this choice is that the vectors $l\lambda_j$ are mutually B_k conjugate, since

$$L_k\lambda - 1 B_k L_k\lambda - T = D_k,$$

and D_k is diagonal. This choice of $\delta\lambda_j$ is slightly more expensive since it involves the solution of n triangular systems of equations on each iteration. Note that, as in *PARALLEL I*, on the $k\lambda th$ iteration, $k \geq 1$,

$$\|\delta\lambda_j\|_2 = \mu \|\mathbf{x}\lambda_k - \mathbf{x}\lambda_{k-1}\|_2, j = 1, 2, \dots, n.$$

The results of Table 1 are obtained using the value $\mu = 10\lambda - 2$ in (4.3).

Table 1 includes the number of function evaluations and the number of iterations required to satisfy the convergence condition. *** indicates that the algorithm fails to satisfy the

convergence condition after 400 function evaluations. The starting values (initial point) are given in Table 1, except for the Mancino function for which the starting values are given in Shanno and Phua (1978b).

These numerical results show that the parallel projected variable metric algorithms, *PARALLEL I* and *PARALLEL II*, converge in less iterations (for some problems considerably less iterations) than the corresponding projected quasi-Newton algorithm. Of course each iteration of the parallel algorithms requires the evaluation of the gradient vector at the n displaced points ; we are assuming that a parallel MIMD computer will allow these gradient vectors to be evaluated simultaneously (indeed the gradient vectors could be evaluated concurrently with the line search of the previous iteration using the *speculative evaluation* ideas of Schnabel (1987)).

Choosing the displacement directions as the normalised columns of $L\lambda - T$, *PARALLEL II*, results in an algorithm which is somewhat more efficient (in terms of iterations) than *PARALLEL I*, which chooses the displacement directions as the co-ordinate directions. *PARALLEL II* requires the solution of n triangular systems of linear equations on each iteration; again a parallel MIMD computer will allow each of these triangular systems to be solved concurrently on the separate processors.

5 Conclusions

One of the major reservations about the parallel variable metric algorithm of Straeter (1965) is its use of the symmetric rank one (*SR1*) updating formula, which allows quadratic termination of the algorithm to be established. In this paper we have generalized Straeter's algorithm to use a projected symmetric rank two updating formula (Davidon (1975)) and have thus developed a family of parallel projected variable metric algorithms. These algorithms avoid the use of the *SR1* updating formula, yet retain the quadratic termination property of Straeter's algorithm.

Initial numerical testing, on a serial computer, indicates that these new parallel algorithms are more efficient (in terms of number of iterations required) than existing serial variable metric algorithms. For some problems, such as the extended Rosenbrock function of dimension 20, the parallel algorithms are considerably more efficient. For this reduced number of iterations to result in an algorithm which is more efficient (in terms of execution time) on a parallel computer depends on the assumption that the cost of function and gradient vector evaluations dominate all other costs of the algorithm.

The new algorithm can exploit parallel computing capabilities to evaluate the displaced gradient vectors; however it is unclear that the sequence of projected rank two updates could

exploit parallelism. The implementation and performance of the new parallel algorithms on a local memory MIMD computer will be reported in a separate paper.

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FUNCTION Initial point	PARALLEL I		PARALLEL II		PROJECTED	
	Iterations	Function evaluations	Iterations	Function evaluations	Iterations	Function evaluations
Rosenbrock 2						
(-1.2,1)	21	22	18	21	35	50
(2,-2)	16	17	15	18	44	62
(-3.635,5.621)	32	34	31	42	27	41
(6.39,-0.221)	35	40	36	48	56	81
(1.489,-2.547)	13	14	12	14	34	52
Rosenbrock 20						
(-1.2,1,...)	23	29	27	37	150	233
(2,-2,...)	37	126	31	50	124	205
(-3.635,5.621,...)	64	170	54	164	99	166
(6.39,-0.221,...)	118	313	64	170	***	***
(1.489,-2.547,...)	22	43	18	41	138	227
Wood 4						
(-3,-1,-3,-1)	37	42	35	48	33	59
(-3,1,-3,1)	38	50	32	41	34	61
(-1.2,1,-1.2,1)	33	41	32	40	70	106
(-1.2,1,1.2,1)	21	26	19	22	46	69
Oren 20						
(1,1,...,1)	43	43	43	43	96	201
Powell 4						
(-3,-1,0,1)	47	48	42	42	72	87
Mancino 10	4	4	4	4	13	62
Mancino 20	5	5	4	4	29	127
Mancino 30	5	5	5	5	33	164

Table 1: Numerical Performance of Parallel variable metric algorithms





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